# Package 'rsbml'

July 3, 2025
<b>Version</b> 2.66.0
Title R support for SBML, using libsbml
Author Michael Lawrence <michafla@gene.com></michafla@gene.com>
<b>Depends</b> R (>= 2.6.0), BiocGenerics (>= 0.3.2), methods, utils
Imports BiocGenerics, graph, utils
SystemRequirements libsbml (==5.10.2)
Maintainer Michael Lawrence <michafla@gene.com></michafla@gene.com>
<b>Description</b> Links R to libsbml for SBML parsing, validating output, provides an S4 SBML DOM, converts SBML to R graph objects. Optionally links to the SBML ODE Solver Library (SOSLib) for simulating models.
License Artistic-2.0
URL http://www.sbml.org
biocViews GraphAndNetwork, Pathways, Network
git_url https://git.bioconductor.org/packages/rsbml
git_branch RELEASE_3_21
git_last_commit 5e15338
git_last_commit_date 2025-04-15
Repository Bioconductor 3.21
Date/Publication 2025-07-02
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AlgebraicRule-class SBML type "AlgebraicRule

# **Description**

Expresses equations that are not assignments nor rates of change.

#### Instantiation

Objects can be created by calls of the form new("AlgebraicRule", ...).

# **Slots**

math: Object of class "expression" specifying the equation.

metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.

notes: Object of class "character" containing user-readable XHTML notes about an element.

annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.

cvTerms: Object of class "list" containing instances of CVTerm associated with this element.

sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

# **Extends**

```
Class "Rule", directly. Class "SBase", by class "Rule", distance 2.
```

# Methods

No methods defined with class "AlgebraicRule" in the signature.

## Author(s)

Michael Lawrence

```
http://sbml.org/documents/
```

AssignmentRule-class SBML type "AssignmentRule"

# **Description**

An equation that assigns a value to the quantity of a Species, the size of a Compartment or the value of a Parameter.

#### Instantiation

Objects can be created by calls of the form new("AssignmentRule", ...).

#### **Slots**

```
variable: Object of class "character" naming the variable (the id of a Species, Compartment or Parameter) to set.
```

type: Object of class "character", deprecated.

math: Object of class "expression" specifying the equation.

metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.

notes: Object of class "character" containing user-readable XHTML notes about an element.

annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.

cvTerms: Object of class "list" containing instances of CVTerm associated with this element. sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

# Extends

```
Class "Rule", directly. Class "SBase", by class "Rule", distance 2.
```

#### Methods

```
variable signature(object = "AssignmentRule"): gets the variable slot
variable<- signature(object = "AssignmentRule"): sets the variable slot
type signature(object = "AssignmentRule"): gets the type slot
type<- signature(object = "AssignmentRule"): sets the type slot</pre>
```

# Author(s)

Michael Lawrence

```
http://sbml.org/documents/
```

BoundingBox-class 5

BoundingBox-class

SBML type "BoundingBox"

# **Description**

Species the size and position of an SBML layout object.

#### Instantiation

Objects can be created by calls of the form new("BoundingBox", ...).

#### **Slots**

```
id: Object of class "character" uniquely identifying this component. position: Object of class "Point" specifying the position. dimensions: Object of class "Dimensions" specifying the size.
```

metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.

notes: Object of class "character" containing user-readable XHTML notes about an element.

annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.

cvTerms: Object of class "list" containing instances of CVTerm associated with this element. sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

#### **Extends**

```
Class "SBase", directly.
```

# Methods

```
id signature(object = "BoundingBox"): gets the id slot
id<- signature(object = "BoundingBox"): sets the id slot
dimensions signature(object = "BoundingBox"): gets the dimensions slot
dimensions<- signature(object = "BoundingBox"): sets the dimensions slot
position signature(object = "BoundingBox"): gets the position slot
position<- signature(object = "BoundingBox"): sets the position slot</pre>
```

#### Author(s)

Michael Lawrence

```
http://projects.villa-bosch.de/bcb/sbml
```

6 Compartment-class

Compartment-class

SBML type "Compartment"

# **Description**

A bounded space that contains Species.

#### Instantiation

Objects can be created by calls of the form new("Compartment", ...).

#### **Slots**

```
id: Object of class "character" uniquely identifying this component.
```

name: Object of class "character" naming this component.

spatialDimensions: Object of class "integer" indicating the number of dimensions (0, 1, 2, or 3)

size: Object of class "numeric" indicating the size in the given units.

units: Object of class "character" indicating the units (built-in or the id of a UnitDefinition).

outside: Object of class "character" identifying the compartment containing this compartment.

constant: Object of class "logical" indicating whether the size changes during simulation.

metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.

notes: Object of class "character" containing user-readable XHTML notes about an element.

annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.

cvTerms: Object of class "list" containing instances of CVTerm associated with this element.

sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

#### **Extends**

```
Class "SBase", directly.
```

## Methods

```
id signature(object = "Compartment"): gets the id slot
id<- signature(object = "Compartment"): sets the id slot
name signature(object = "Compartment"): gets the name slot
name<- signature(object = "Compartment"): sets the name slot
constant signature(object = "Compartment"): gets the constant slot</pre>
```

```
constant<- signature(object = "Compartment"): sets the constant slot
outside signature(object = "Compartment"): gets the outside slot
outside<- signature(object = "Compartment"): sets the outside slot
size signature(object = "Compartment"): gets the size slot
size<- signature(object = "Compartment"): sets the size slot
units signature(object = "Compartment"): gets the constant slot
units<- signature(object = "Compartment"): sets the constant slot
spatialDimensions signature(object = "Compartment"): gets the spatialDimensions slot
spatialDimensions<- signature(object = "Compartment"): sets the spatialDimensions slot</pre>
```

## Author(s)

Michael Lawrence

#### References

http://sbml.org/documents/

CompartmentGlyph-class

SBML type "CompartmentGlyph"

# **Description**

A glyph representing a Compartment.

#### Instantiation

Objects can be created by calls of the form new("CompartmentGlyph", ...).

# Slots

compartment: Object of class "character" identifying the compartment this glyph represents.

id: Object of class "character" uniquely identifying this component.

boundingBox: Object of class "BoundingBox" describing the position and size of the graphical object.

metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.

notes: Object of class "character" containing user-readable XHTML notes about an element.

annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.

cvTerms: Object of class "list" containing instances of CVTerm associated with this element. sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

# **Extends**

Class "GraphicalObject", directly. Class "SBase", by class "GraphicalObject", distance 2.

#### Methods

```
compartment signature(object = "CompartmentGlyph"): gets the compartment slot
compartment<- signature(object = "CompartmentGlyph"): sets the compartment slot</pre>
```

# Author(s)

Michael Lawrence

#### References

http://projects.villa-bosch.de/bcb/sbml

CompartmentType-class SBML Type "CompartmentType"

# **Description**

Declares a type of Compartment. Compartments with the same type are logically similar.

# **Objects from the Class**

Objects can be created by calls of the form new("CompartmentType", ...).

# **Slots**

id: Object of class "character" uniquely identifying this component.

name: Object of class "character" naming this component.

metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.

notes: Object of class "character" containing user-readable XHTML notes about an element.

annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.

cvTerms: Object of class "list" containing instances of CVTerm associated with this element.

sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

# Extends

Class "SBase", directly.

# Methods

```
id signature(object = "CompartmentType"): gets the id slot
id<- signature(object = "CompartmentType"): sets the id slot
name signature(object = "CompartmentType"): gets the name slot
name<- signature(object = "CompartmentType"): sets the name slot</pre>
```

# Note

Requires libsbml >= 3.0

## Author(s)

Michael Lawrence

#### References

http://sbml.org/documents/

#### See Also

Compartment

CompartmentVolumeRule-class

SBML type "CompartmentVolumeRule"

# **Description**

**Obsolete** way to assign a volume to a Compartment.

# Instantiation

Objects can be created by calls of the form new("CompartmentVolumeRule", ...).

# **Slots**

```
compartment: Object of class "character" identifying the compartment variable: Object of class "character", ignored.

type: Object of class "character", deprecated.

math: Object of class "expression" specifying the equation.

metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.
```

notes: Object of class "character" containing user-readable XHTML notes about an element.

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annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.

cvTerms: Object of class "list" containing instances of CVTerm associated with this element. sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

#### **Extends**

Class "AssignmentRule", directly. Class "Rule", by class "AssignmentRule", distance 2. Class "SBase", by class "AssignmentRule", distance 3.

#### Methods

```
compartment signature(object = "CompartmentVolumeRule"): gets the compartment slot
compartment<- signature(object = "CompartmentVolumeRule"): sets the compartment slot</pre>
```

#### Author(s)

Michael Lawrence

#### References

```
http://sbml.org/documents/
```

Constraint-class

SBML Type "Constraint"

# **Description**

A constraint that must be continuously satisfied throughout the simulation of a model. Once a constraint is no longer met, the simulation must halt.

# **Objects from the Class**

Objects can be created by calls of the form new("Constraint", ...).

# **Slots**

math: Object of class "expression" that evaluates to FALSE if the constraint is not satisfied, otherwise evaluates to TRUE.

message: Object of class "character", formatted in XHTML, that is displayed to the user by an application when the constraint is not satisfied.

metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.

notes: Object of class "character" containing user-readable XHTML notes about an element.

CubicBezier-class 11

annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.

cvTerms: Object of class "list" containing instances of CVTerm associated with this element.

sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

# **Extends**

```
Class "SBase", directly.
```

#### Methods

```
math signature(domain = "Constraint"): gets the math slot.
math<- signature(object = "Constraint"): sets the math slot.
msg signature(domain = "Constraint"): gets the msg slot.
msg<- signature(object = "Constraint"): sets the msg slot.</pre>
```

#### Note

Requires libsbml >= 3.0

# Author(s)

Michael Lawrence

#### References

```
http://sbml.org/documents/
```

CubicBezier-class

SBML type "CubicBezier"

# **Description**

A cubic bezier curve in an SBML layout.

# Instantiation

Objects can be created by calls of the form new("CubicBezier", ...).

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#### Slots

basePoint1: Object of class "Point" indicating the position of the base point closest to the starting point.

basePoint2: Object of class "Point" indicating the position of the base point farthest from the starting point.

```
start: Object of class "Point" ~~
end: Object of class "Point" ~~
```

metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.

notes: Object of class "character" containing user-readable XHTML notes about an element.

annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.

cvTerms: Object of class "list" containing instances of CVTerm associated with this element.

sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

#### **Extends**

```
Class "LineSegment", directly. Class "SBase", by class "LineSegment", distance 2.
```

# Methods

```
basePoint1 signature(object = "CubicBezier"): gets the basePoint1 slot
basePoint1<- signature(object = "CubicBezier"): sets the basePoint1 slot
basePoint2 signature(object = "CubicBezier"): gets the basePoint2 slot
basePoint2<- signature(object = "CubicBezier"): sets the basePoint2 slot</pre>
```

# Author(s)

Michael Lawrence

```
http://projects.villa-bosch.de/bcb/sbml
```

Curve-class 13

Curve-class

SBML type "Curve"

# **Description**

A curve (list of line segments) in an SBML layout.

#### Instantiation

Objects can be created by calls of the form new("Curve", ...).

#### **Slots**

curveSegments: Object of class "list" containing the LineSegments that compose the curve.

metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.

notes: Object of class "character" containing user-readable XHTML notes about an element.

annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.

cvTerms: Object of class "list" containing instances of CVTerm associated with this element.

sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

## **Extends**

```
Class "SBase", directly.
```

#### Methods

```
curveSegments signature(object = "Curve"): gets the curveSegments slot
curveSegments<- signature(object = "Curve"): sets the curveSegments slot</pre>
```

# Author(s)

Michael Lawrence

```
http://projects.villa-bosch.de/bcb/sbml
```

14 CVTerm-class

CVTerm-class

SBML Type "CVTerm"

# **Description**

A MIRIAM annotation, consisting of a qualifier ("model", "biological" or something else) and a resource (URI).

## **Objects from the Class**

Objects can be created by calls of the form new("CVTerm", ...).

#### **Slots**

qualifierType: Object of class "character" specifying the type of qualifier for this term. Types "model" and "biological" have special meaning, but any string may be specified.

modelQualifierType: Object of class "character" specifying the type of model qualifier, if qualifierType is set to "model". Types "is" and "isDescribedBy" are formally defined in MIRIAM, but any string may be specified.

biologicalQualifierType: Object of class "character" specifying the type of biological qualifier, if qualifierType is set to "biological". Types "is", "hasPart", "isPartOf", "isVersionOf", "hasVersion", "isHomologTo", and "isDescribedBy" are formally defined in MIRIAM, though any string may be specified.

resources: Object of class "character" specifying a URI that identifies some resource related an SBML element by the qualifier.

#### Methods

modelQualifierType signature(object = "CVTerm"): gets the modelQualifierType slot.

modelQualifierType<- signature(object = "CVTerm"): sets the modelQualifierType slot.

qualifierType signature(object = "CVTerm"): gets the qualifierType slot.

qualifierType<- signature(object = "CVTerm"): sets the qualifierType slot.

**resources** signature(object = "CVTerm"): gets the resources slot.

resources<- signature(object = "CVTerm"): sets the resources slot.</pre>

## Author(s)

Michael Lawrence

#### References

http://sbml.org/documents/

Delay-class 15

Delay-class

SBML Type "Delay"

# **Description**

The length of time between the Triggering of an Event and the execution of its EventAssignments.

# **Objects from the Class**

Objects can be created by calls of the form new("Delay", ...).

# Slots

math: Object of class "expression" that evaluates to a quantity of time.

metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.

notes: Object of class "character" containing user-readable XHTML notes about an element.

annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.

cvTerms: Object of class "list" containing instances of CVTerm associated with this element. sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

# **Extends**

```
Class "SBase", directly.
```

# Methods

```
math signature(domain = "Delay"): gets the math slot.
math<- signature(object = "Delay"): sets the math slot.</pre>
```

# Note

Requires libsbml >= 3.0

#### Author(s)

Michael Lawrence

# References

```
http://sbml.org/documents/
```

# See Also

**Event** 

16 describe

describe Describing objects

# Description

Each class in the SBML DOM extends the Describable class and thus has a describe method, which describes an object with a short string. This is used by the show method to output terse textual representations of the DOM.

# Usage

```
describe(object, ...)
```

# Arguments

object The object to be described.

... Additional arguments for methods.

# Value

A short textual (string) representation of object.

# Describable objects

An object that extends Describable has a method for the describe generic, and by default Describable objects are shown by printing the output of describe. Note that Describable is a virtual tag class, no objects may be created from it.

# Describable methods

```
show signature(object = "Describable"): outputs the return value of describe.
```

# Author(s)

Michael Lawrence

Dimensions-class 17

Dimensions-class

SBML type "Dimensions"

# **Description**

Holds the size of an SBML layout object.

#### Instantiation

Objects can be created by calls of the form new("Dimensions", ...).

#### **Slots**

```
width: Object of class "numeric" indicating the width, in pixels
height: Object of class "numeric" indicating the height, in pixels
depth: Object of class "numeric" indicating the depth, in pixels
metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This
links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element,
but is usually placed inside the annotation element.
notes: Object of class "character" containing user-readable XHTML notes about an element.
annotation: Object of class "character" containing additional machine-readable information
about an element, usually as RDF, such as BioPAX. This is where application-specific data
belongs.
cvTerms: Object of class "list" containing instances of CVTerm associated with this element.
```

sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

#### **Extends**

```
Class "SBase", directly.
```

# Methods

```
depth signature(object = "Dimensions"): gets the depth slot
depth<- signature(object = "Dimensions"): sets the depth slot
height signature(object = "Dimensions"): gets the height slot
height<- signature(object = "Dimensions"): sets the height slot
width signature(object = "Dimensions"): gets the width slot
width<- signature(object = "Dimensions"): sets the width slot</pre>
```

#### Author(s)

Michael Lawrence

```
http://projects.villa-bosch.de/bcb/sbml
```

18 Event-class

Event-class

SBML type "Event"

# Description

Description of a instantaneous, discontinuous change in the model state.

#### Instantiation

Objects can be created by calls of the form new("Event", ...).

#### Slots

id: Object of class "character" uniquely identifying this component.

name: Object of class "character" naming this component.

trigger: Object of class "expression" that evaluates to TRUE when the event is to be fired.

eventDelay: Object of class "expression" that evaluates to the time until execution of this event after it has been fired.

timeUnits: Object of class "character" identifying the units of the delay.

eventAssignments: Object of class "list" containing EventAssignments that are performed at execution.

useValuesFromTriggerTime: Object of class "logical". If FALSE, the event is evaluated after the delay, rather than when the event is executed.

metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.

notes: Object of class "character" containing user-readable XHTML notes about an element.

annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.

cvTerms: Object of class "list" containing instances of CVTerm associated with this element.

sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

# **Extends**

```
Class "SBase", directly.
```

#### Methods

```
id signature(object = "Event"): gets the id slot
id<- signature(object = "Event"): sets the id slot
name signature(object = "Event"): gets the name slot
name<- signature(object = "Event"): sets the name slot</pre>
```

EventAssignment-class

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```
timeUnits signature(object = "Event"): gets the timeUnits slot
timeUnits<- signature(object = "Event"): sets the timeUnits slot
eventDelay signature(x = "Event"): ...
eventDelay<- signature(object = "Event"): sets the delay slot
eventAssignments signature(object = "Event"): gets the eventAssignments slot
eventAssignments<- signature(object = "Event"): sets the eventAssignments slot
trigger signature(object = "Event"): gets the trigger slot
trigger<- signature(object = "Event"): sets the trigger slot</pre>
```

## Author(s)

Michael Lawrence

#### References

http://sbml.org/documents/

EventAssignment-class SBML type "EventAssignment"

# Description

As part of an event, assigns a value to the quantity of a Species, the size of a Compartment or the value of a Parameter.

#### Instantiation

Objects can be created by calls of the form new("EventAssignment", ...).

# Slots

```
variable: Object of class "character" ~~
```

math: Object of class "expression" that evaluates to the value to assign.

metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.

notes: Object of class "character" containing user-readable XHTML notes about an element.

annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.

cvTerms: Object of class "list" containing instances of CVTerm associated with this element.

sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

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# **Extends**

```
Class "SBase", directly.
```

#### Methods

```
math signature(object = "EventAssignment"): gets the math slot
math<- signature(object = "EventAssignment"): sets the math slot
variable signature(object = "EventAssignment"): gets the variable slot
variable<- signature(object = "EventAssignment"): sets the variable slot</pre>
```

#### Author(s)

Michael Lawrence

# References

http://sbml.org/documents/

Experiment-class

Experiment

# **Description**

This class is an abstraction for an experiment, e.g. in a simulation. An experiment consists of a ExperimentProtocol, ExperimentDesign, ExperimentSubject and ExperimentResult.

# **Objects from the Class**

A virtual Class: No objects may be created from it.

# **Slots**

protocol: Object of empty virtual class ExperimentProtocol, how the experiment was or is to be performed.

design: Object of empty virtual class ExperimentDesign, the design of the experiment.

subject: Object of empty virtual class ExperimentSubject, the object being observed by the experiment.

result: Object of empty virtual class ExperimentResult, the result of the experiment.

FunctionDefinition-class 21

#### Methods

```
design signature(object = "Experiment"): Gets the design slot.
design<- signature(object = "Experiment"): Sets the design slot.
protocol signature(object = "Experiment"): Gets the protocol slot.
protocol<- signature(object = "Experiment"): Sets the protocol slot.
result signature(object = "Experiment"): Gets the result slot.
result<- signature(object = "Experiment"): Sets the result slot.
subject signature(object = "Experiment"): Gets the subject slot.
subject<- signature(object = "Experiment"): Sets the subject slot.</pre>
```

#### Author(s)

Michael Lawrence

#### See Also

SOSExperiment, an implementation that simulates SBML modules using the SBML ODE Solver library.

FunctionDefinition-class

SBML type "FunctionDefinition"

# **Description**

Identifies a mathematical expression so that it may be referenced in other expressions.

# Instantiation

Objects can be created by calls of the form new("FunctionDefinition", ...).

# **Slots**

id: Object of class "character" uniquely identifying this component.

name: Object of class "character" naming this component.

math: Object of class "expression" that defines the function.

metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.

notes: Object of class "character" containing user-readable XHTML notes about an element.

annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.

cvTerms: Object of class "list" containing instances of CVTerm associated with this element. sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

#### **Extends**

```
Class "SBase", directly.
```

#### Methods

```
id signature(object = "FunctionDefinition"): gets the id slot
id<- signature(object = "FunctionDefinition"): sets the id slot
name signature(object = "FunctionDefinition"): gets the name slot
name<- signature(object = "FunctionDefinition"): sets the name slot
math signature(object = "FunctionDefinition"): gets the math slot
math<- signature(object = "FunctionDefinition"): sets the math slot</pre>
```

## Author(s)

Michael Lawrence

#### References

```
http://sbml.org/documents/
```

GraphicalObject-class SBML type "GraphicalObject"

# **Description**

The base class for graphical objects (e.g. glyphs) in SBML layouts.

#### Instantiation

Objects can be created by calls of the form new("GraphicalObject", ...).

# **Slots**

id: Object of class "character" uniquely identifying this component.

boundingBox: Object of class "BoundingBox" describing the position and size of the graphical object.

metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.

notes: Object of class "character" containing user-readable XHTML notes about an element.

annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.

cvTerms: Object of class "list" containing instances of CVTerm associated with this element. sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

InitialAssignment-class

#### 23

# **Extends**

```
Class "SBase", directly.
```

#### Methods

```
id signature(object = "GraphicalObject"): gets the id slot
id<- signature(object = "GraphicalObject"): sets the id slot
boundingBox signature(object = "GraphicalObject"): gets the boundingBox slot
boundingBox<- signature(object = "GraphicalObject"): sets the boundingBox slot</pre>
```

# Author(s)

Michael Lawrence

#### References

```
http://projects.villa-bosch.de/bcb/sbml
```

```
InitialAssignment-class
```

SBML Type "InitialAssignment"

# Description

Calculates the value of a symbol when the model is initialized.

# **Objects from the Class**

Objects can be created by calls of the form new("InitialAssignment", ...).

# Slots

```
symbol: Object of class "character" to which the value is assigned.
```

math: Object of class "expression" that evaluates to the assigned value.

metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.

notes: Object of class "character" containing user-readable XHTML notes about an element.

annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.

```
cvTerms: Object of class "list" containing instances of CVTerm associated with this element.
```

sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

24 KineticLaw-class

# **Extends**

```
Class "SBase", directly.
```

#### Methods

```
math signature(object = "InitialAssignment"): gets the math slot.
math<- signature(object = "InitialAssignment"): sets the math slot.
symbol signature(object = "InitialAssignment"): gets the symbol slot.
symbol<- signature(object = "InitialAssignment"): sets the symbol slot.</pre>
```

## Note

Requires libsbml >= 3.0

## Author(s)

Michael Lawrence

# References

```
http://sbml.org/documents/
```

#### See Also

AssignmentRule, which can set a value at any time but cannot set constants.

KineticLaw-class

SBML type "KineticLaw"

# Description

Describes the rate of a Reaction.

# Instantiation

Objects can be created by calls of the form new("KineticLaw", ...).

# **Slots**

```
math: Object of class "expression" defining the rate of the reaction.
```

parameters: Object of class "list" containing Parameters that may be used in math. The names of the list correspond to the IDs of the elements.

```
timeUnits: Object of class "character" indicating the units for time.
```

substanceUnits: Object of class "character" indicating the units for substance.

Layout-class 25

metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.

notes: Object of class "character" containing user-readable XHTML notes about an element.

annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.

cvTerms: Object of class "list" containing instances of CVTerm associated with this element. sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

#### Extends

```
Class "SBase", directly.
```

#### Methods

```
math signature(object = "KineticLaw"): gets the math slot
math<- signature(object = "KineticLaw"): sets the math slot
substanceUnits signature(object = "KineticLaw"): gets the substanceUnits slot
substanceUnits<- signature(object = "KineticLaw"): sets the substanceUnits slot
timeUnits signature(object = "KineticLaw"): gets the timeUnits slot
timeUnits<- signature(object = "KineticLaw"): sets the timeUnits slot
parameters signature(object = "KineticLaw"): gets the parameters slot
parameters<- signature(object = "KineticLaw"): sets the parameters slot</pre>
```

## Author(s)

Michael Lawrence

#### References

```
http://sbml.org/documents/
```

Layout-class

SBML type "Layout"

# **Description**

Contains the glyphs and other graphical objects that compose an SBML layout. Layouts are not part of the core SBML specification. See the reference for the SBML layout extension specification.

# Instantiation

Objects can be created by calls of the form new("Layout", ...).

26 Layout-class

#### **Slots**

id: Object of class "character" uniquely identifying this component.

dimensions: Object of class "Dimensions" specifing the size of the layout.

compartmentGlyphs: Object of class "list" containing the CompartmentGlyphs. The names of the list correspond to the IDs of the elements.

speciesGlyphs: Object of class "list" containing the SpeciesGlyphs. The names of the list correspond to the IDs of the elements.

reactionGlyphs: Object of class "list" containing the ReactionGlyphs. The names of the list correspond to the IDs of the elements.

textGlyphs: Object of class "list" containing the TextGlyphs. The names of the list correspond to the IDs of the elements.

additionalGraphicalObjects: Object of class "list" containing the additional GraphicalObjects that are not bound to any model component. The names of the list correspond to the IDs of the elements.

metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.

notes: Object of class "character" containing user-readable XHTML notes about an element.

annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.

cvTerms: Object of class "list" containing instances of CVTerm associated with this element.

sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

#### **Extends**

```
Class "SBase", directly.
```

# Methods

LineSegment-class 27

```
speciesGlyphs signature(object = "Layout"): gets the speciesGlyphs slot
speciesGlyphs<- signature(object = "Layout"): sets the speciesGlyphs slot
textGlyphs signature(object = "Layout"): gets the textGlyphs slot
textGlyphs<- signature(object = "Layout"): sets the textGlyphs slot</pre>
```

# Author(s)

Michael Lawrence

#### References

```
http://projects.villa-bosch.de/bcb/sbml
```

LineSegment-class

SBML type "LineSegment"

# **Description**

Describes a simple A-B line.

# Instantiation

Objects can be created by calls of the form new("LineSegment", ...).

# **Slots**

start: Object of class "Point" indicating the start position.

end: Object of class "Point" indicating the end position.

metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.

notes: Object of class "character" containing user-readable XHTML notes about an element.

annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.

 ${\tt cvTerms:} \ \ Object \ of \ class \ "list" \ containing \ instances \ of \ {\tt cvTerm} \ associated \ with \ this \ element.$ 

sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

#### **Extends**

```
Class "SBase", directly.
```

28 math

# Methods

```
end signature(x = "LineSegment"): ...
end<- signature(object = "LineSegment"): sets the end slot
start signature(x = "LineSegment"): ...
start<- signature(object = "LineSegment"): sets the start slot</pre>
```

# Author(s)

Michael Lawrence

#### References

http://projects.villa-bosch.de/bcb/sbml

math

MathML Utilities

# Description

Each of these functions implements a trigonometry function found in the MathML specification but not found in base R. These are all simple wrappers around existing R trig functions.

# Usage

acot(x)
acoth(x)
acsc(x)
acsch(x)
asec(x)
asech(x)
cot(x)
coth(x)
csc(x)
csch(x)
sec(x)
sech(x)

# **Arguments**

Х

The numeric value(s) for the trigonometry operation

#### Value

A numeric vector, the same length as x.

# Author(s)

Michael Lawrence

Model-class 29

Model-class SBML type "Model"

# **Description**

The central SBML element. Contains the Species, Reactions, Compartments and other components of the model. See the SBML specification, at the reference, for further details.

#### Instantiation

Objects can be created by calls of the form new("Model", ...).

#### **Slots**

id: Object of class "character" uniquely identifying this component.

name: Object of class "character" naming this component.

functionDefinitions: Object of class "list" containing FunctionDefinitions. The names of the list correspond to the IDs of the elements.

unitDefinitions: Object of class "list" containing UnitDefinitions. The names of the list correspond to the IDs of the elements.

compartments: Object of class "list" containing Compartments. The names of the list correspond to the IDs of the elements.

species: Object of class "list" containing Speciess. The names of the list correspond to the IDs of the elements.

parameters: Object of class "list" containing Parameters. The names of the list correspond to the IDs of the elements.

rules: Object of class "list" containing Rules.

reactions: Object of class "list" containing Reactions. The names of the list correspond to the IDs of the elements.

events: Object of class "list" containing Events. The names of the list correspond to the IDs of the elements.

layouts: Object of class "list" containing Layouts. The names of the list correspond to the IDs of the elements.

speciesTypes: Object of class "list" containing SpeciesTypes. The names of the list correspond to the IDs of the elements.

compartmentTypes: Object of class "list" containing CompartmentTypes. The names of the list correspond to the IDs of the elements.

constraints: Object of class "list" containing Constraints. The names of the list correspond to the IDs of the elements.

initialAssignments: Object of class "list" containing InitialAssignments.

modelHistory: Object of class ModelHistory recording the history of the model.

30 Model-class

metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.

notes: Object of class "character" containing user-readable XHTML notes about an element.

annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.

cvTerms: Object of class "list" containing instances of CVTerm associated with this element. sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

#### Extends

```
Class "SBase", directly.
```

#### Methods

```
id signature(object = "Model"): gets the id slot
id<- signature(object = "Model"): sets the id slot</pre>
name signature(object = "Model"): gets the name slot
name<- signature(object = "Model"): sets the name slot</pre>
compartments signature(object = "Model"): gets the compartments slot
compartments<- signature(object = "Model"): sets the compartments slot</pre>
events signature(object = "Model"): gets the events slot
events<- signature(object = "Model"): sets the events slot
functionDefinitions signature(object = "Model"): gets the functionDefinitions slot
functionDefinitions<- signature(object = "Model"): sets the functionDefinitions slot
layouts signature(object = "Model"): gets the layouts slot
layouts<- signature(object = "Model"): sets the layouts slot</pre>
parameters signature(object = "Model"): gets the parameters slot
parameters<- signature(object = "Model"): sets the parameters slot</pre>
species signature(object = "Model"): gets the species slot
species<- signature(object = "Model"): sets the species slot</pre>
reactions signature(object = "Model"): gets the reactions slot
reactions<- signature(object = "Model"): sets the reactions slot</pre>
rules signature(object = "Model"): gets the rules slot
rules<- signature(object = "Model"): sets the rules slot
unitDefinitions signature(object = "Model"): gets the unitDefinitions slot
unitDefinitions<- signature(object = "Model"): sets the unitDefinitions slot</pre>
compartmentTypes signature(object = "Model"): gets the compartmentTypes slot
compartmentTypes<- signature(object = "Model"): sets the compartmentTypes slot</pre>
```

ModelCreator-class 31

```
constraints signature(object = "Model"): gets the constraints slot
constraints<- signature(object = "Model"): sets the constraints slot
initialAssignments signature(object = "Model"): gets the initialAssignments slot
initialAssignments<- signature(object = "Model"): sets the initialAssignments slot
speciesTypes signature(object = "Model"): gets the speciesTypes slot
speciesTypes<- signature(object = "Model"): sets the speciesTypesslot
modelHistory signature(object = "Model"): gets the modelHistory slot
modelHistory<- signature(object = "Model"): sets the modelHistory slot
stoichiometryMatrix signature(object = "Model"): calculates the stoichiometry matrix of the
model</pre>
```

# Author(s)

Michael Lawrence

#### References

http://sbml.org/documents/

ModelCreator-class

SBML Type "ModelCreator"

# Description

Information, such as name, email and organization, about a creator of an SBML model.

# **Objects from the Class**

Objects can be created by calls of the form new("ModelCreator", ...).

# **Slots**

```
familyName: Object of class "character" specifying the family name of the creator.

givenName: Object of class "character" specifying the given name of the creator.

email: Object of class "character" specifying the email address of the creator.

organization: Object of class "character" specifying the name of the organization to which the creator belongs.
```

32 ModelHistory-class

# Methods

```
email signature(object = "ModelCreator"): gets the email slot.
email<- signature(object = "ModelCreator"): sets the email<- slot.
familyName signature(object = "ModelCreator"): gets the familyName slot.
familyName<- signature(object = "ModelCreator"): sets the familyName<- slot.
givenName signature(object = "ModelCreator"): gets the givenName slot.
givenName<- signature(object = "ModelCreator"): sets the givenName<- slot.
organization signature(object = "ModelCreator"): gets the organization slot.
organization<- signature(object = "ModelCreator"): sets the organization<- slot.</pre>
```

# Author(s)

Michael Lawrence

#### References

http://sbml.org/documents/

ModelHistory-class

SBML Type "ModelHistory"

# **Description**

Stores the history of an SBML model, including the created/modified dates and the creators.

# **Objects from the Class**

Objects can be created by calls of the form new("ModelHistory", ...).

# Slots

```
createdDate: Object of class "character" representing the date/time of creation, in W3CDTF format: YYYY-MM-DDThh:mm:ssTZD, e.g. "1997-07-16T19:20:30+01:00".
```

modifiedDate: Object of class "character" representing the date/time of last modification, in W3CDTF format: YYYY-MM-DDThh:mm:ssTZD, e.g. "1997-07-16T19:20:30+01:00".

creators: Object of class "list" of instances of ModelCreator, one for each creator of the model.

#### Methods

## Author(s)

Michael Lawrence

#### References

```
http://sbml.org/documents/
```

ModifierSpeciesReference-class

SBML type "ModifierSpeciesReference"

# Description

Identifies a Species that modifies the parent Reaction.

# Instantiation

Objects can be created by calls of the form new("ModifierSpeciesReference", ...).

#### **Slots**

```
    id: Object of class "character" uniquely identifying this component.
    species: Object of class "character" identifying the Species being referenced.
    metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.
```

notes: Object of class "character" containing user-readable XHTML notes about an element.

34 Parameter-class

annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.

cvTerms: Object of class "list" containing instances of CVTerm associated with this element. sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

#### **Extends**

Class "SimpleSpeciesReference", directly. Class "SBase", by class "SimpleSpeciesReference", distance 2.

#### Methods

No methods defined with class "ModifierSpeciesReference" in the signature.

# Author(s)

Michael Lawrence

#### References

http://sbml.org/documents/

Parameter-class

SBML type "Parameter"

# **Description**

Declares a variable to be used in a mathematical expression.

## Instantiation

Objects can be created by calls of the form new("Parameter", ...).

# **Slots**

id: Object of class "character" uniquely identifying this component.

name: Object of class "character" naming this component.

value: Object of class "numeric" specifying the initial value.

units: Object of class "character" identifying the units.

constant: Object of class "logical" indicating whether the value of this parameter is constant.

metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.

notes: Object of class "character" containing user-readable XHTML notes about an element.

ParameterRule-class 35

annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.

cvTerms: Object of class "list" containing instances of CVTerm associated with this element. sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

# **Extends**

```
Class "SBase", directly.
```

#### Methods

```
id signature(object = "Parameter"): gets the id slot
id<- signature(object = "Parameter"): sets the id slot
name signature(object = "Parameter"): gets the name slot
name<- signature(object = "Parameter"): sets the name slot
units signature(object = "Parameter"): gets the units slot
units<- signature(object = "Parameter"): sets the units slot
constant signature(object = "Parameter"): gets the constant slot
constant<- signature(object = "Parameter"): sets the constant slot
value signature(object = "Parameter"): gets the value slot
value<- signature(object = "Parameter"): sets the value slot</pre>
```

# Author(s)

Michael Lawrence

# References

```
http://sbml.org/documents/
```

ParameterRule-class

SBML type "ParameterRule"

# **Description**

**Obsolete** rule that controls the value of a Parameter.

## Instantiation

Objects can be created by calls of the form new("ParameterRule", ...).

36 ParameterRule-class

#### **Slots**

```
name: Object of class "character" naming this component.
units: Object of class "character" identifying the units of the assigned value.
variable: Object of class "character", ignored.
type: Object of class "character", deprecated.
math: Object of class "expression" specifying the equation.
metald: Object of class "character" that is an XML ID "described" by an RDF resource. This
```

links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.

notes: Object of class "character" containing user-readable XHTML notes about an element.

annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.

cvTerms: Object of class "list" containing instances of CVTerm associated with this element. sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

#### **Extends**

Class "AssignmentRule", directly. Class "Rule", by class "AssignmentRule", distance 2. Class "SBase", by class "AssignmentRule", distance 3.

# Methods

```
name signature(object = "Parameter"): gets the name slot
name<- signature(object = "Parameter"): sets the name slot
units signature(object = "Parameter"): gets the units slot
units<- signature(object = "Parameter"): sets the units slot
variable signature(object = "Parameter"): gets the variable slot
variable<- signature(object = "Parameter"): sets the variable slot
type signature(object = "Parameter"): gets the type slot
type<- signature(object = "Parameter"): sets the type slot
math signature(object = "Parameter"): gets the math slot
math<- signature(object = "Parameter"): sets the math slot</pre>
```

#### Author(s)

Michael Lawrence

```
http://sbml.org/documents/
```

Point-class 37

Point-class

SBML type "Point"

# **Description**

Specifies a position in 3D space.

## Instantiation

Objects can be created by calls of the form new("Point", ...).

## **Slots**

```
x: Object of class "numeric" indicating the X coordinate
```

- y: Object of class "numeric" indicating the Y coordinate
- z: Object of class "numeric" indicating the Z coordinate

metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.

notes: Object of class "character" containing user-readable XHTML notes about an element.

annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.

cvTerms: Object of class "list" containing instances of CVTerm associated with this element. sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

#### **Extends**

```
Class "SBase", directly.
```

# Methods

```
x signature(object = "Point"): gets the x slot
x<- signature(object = "Point"): sets the x slot
y signature(object = "Point"): gets the y slot
y<- signature(object = "Point"): sets the y slot
z signature(object = "Point"): gets the z slot
z<- signature(object = "Point"): sets the z slot</pre>
```

#### Author(s)

Michael Lawrence

#### References

```
http://projects.villa-bosch.de/bcb/sbml
```

38 RateRule-class

RateRule-class

SBML type "RateRule"

# Description

An equation that describes the rate of change in the quantity of a Species, the size of a Compartment or the value of a Parameter.

#### Instantiation

Objects can be created by calls of the form new("RateRule", ...).

#### **Slots**

variable: Object of class "character" naming the variable (the id of a Species, Compartment or Parameter) being described.

math: Object of class "expression" specifying the equation.

metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.

notes: Object of class "character" containing user-readable XHTML notes about an element.

annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.

cvTerms: Object of class "list" containing instances of CVTerm associated with this element.

sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

#### **Extends**

```
Class "Rule", directly. Class "SBase", by class "Rule", distance 2.
```

#### Methods

```
variable signature(object = "RateRule"): gets the variable slot
variable<- signature(object = "RateRule"): sets the variable slot</pre>
```

# Author(s)

Michael Lawrence

# References

```
http://sbml.org/documents/
```

Reaction-class 39

Reaction-class SBML type "Reaction"

## **Description**

Any transformation, transportation or binding process that changes the quantity of one or more Species.

## Instantiation

Objects can be created by calls of the form new("Reaction", ...).

# Slots

id: Object of class "character" uniquely identifying this component.

name: Object of class "character" naming this component.

reactants: Object of class "list" containing SpeciesReferences specifying the Species that are reactants for this reaction. The names of the list correspond to the IDs of the species.

products: Object of class "list" containing SpeciesReferences specifying the Species that are products for this reaction. The names of the list correspond to the IDs of the species.

modifiers: Object of class "list" containing ModifierSpeciesReferences specifying the Species that are modifiers for this reaction. The names of the list correspond to the IDs of the species.

kineticLaw: Object of class "KineticLaw" that dynamically defines the rate of the reaction.

reversible: Object of class "logical" indicating whether the direction of this reaction is reversible.

fast: Object of class "logical" indicating whether this reaction should be considered instantaneous relative to non-fast reactions.

metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.

notes: Object of class "character" containing user-readable XHTML notes about an element.

annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.

cvTerms: Object of class "list" containing instances of CVTerm associated with this element.

sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

#### **Extends**

Class "SBase", directly.

ReactionGlyph-class

## Methods

```
id signature(object = "Reaction"): gets the id slot
id<- signature(object = "Reaction"): sets the id slot</pre>
name signature(object = "Reaction"): gets the name slot
name<- signature(object = "Reaction"): sets the name slot</pre>
fast signature(object = "Reaction"): gets the fast slot
fast<- signature(object = "Reaction"): sets the fast slot</pre>
kineticLaw signature(object = "Reaction"): gets the kineticLaw slot
kineticLaw<- signature(object = "Reaction"): sets the kineticLaw slot</pre>
modifiers signature(object = "Reaction"): gets the modifiers slot
modifiers<- signature(object = "Reaction"): sets the modifiers slot
products signature(object = "Reaction"): gets the products slot
products<- signature(object = "Reaction"): sets the products slot</pre>
reactants signature(object = "Reaction"): gets the reactants slot
reactants<- signature(object = "Reaction"): sets the reactants slot</pre>
reversible signature(object = "Reaction"): gets the reversible slot
reversible<- signature(object = "Reaction"): sets the reversible slot</pre>
```

## Author(s)

Michael Lawrence

## References

http://sbml.org/documents/

ReactionGlyph-class SBML type "ReactionGlyph"

# Description

A glyph representing a Reaction in the SBML layout.

#### Instantiation

Objects can be created by calls of the form new("ReactionGlyph", ...).

ReactionGlyph-class 41

#### **Slots**

reaction: Object of class "character" identifying the reaction represented by this glyph.

glyphCurve: Object of class "Curve" describing this glyph as a curve (optional).

speciesReferenceGlyphs: Object of class "list" containing SpeciesReferenceGlyphs that represent the SpeciesReferences of the underlying Reaction. The names of the list correspond to the IDs of the elements.

id: Object of class "character" uniquely identifying this component.

boundingBox: Object of class "BoundingBox" describing the position and size of the graphical object.

metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.

notes: Object of class "character" containing user-readable XHTML notes about an element.

annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.

cvTerms: Object of class "list" containing instances of CVTerm associated with this element. sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

#### **Extends**

Class "GraphicalObject", directly. Class "SBase", by class "GraphicalObject", distance 2.

#### Methods

# Author(s)

Michael Lawrence

# References

http://projects.villa-bosch.de/bcb/sbml

42 Rule-class

Rule-class

SBML type "Rule"

# Description

A mathematical equation.

#### Instantiation

A virtual Class: No objects may be created from it.

#### **Slots**

math: Object of class "expression" specifying the equation.

metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.

notes: Object of class "character" containing user-readable XHTML notes about an element.

annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.

cvTerms: Object of class "list" containing instances of CVTerm associated with this element.

sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

## **Extends**

```
Class "SBase", directly.
```

#### Methods

```
math signature(object = "Rule"): gets the math slot
math<- signature(object = "Rule"): sets the math slot</pre>
```

# Author(s)

Michael Lawrence

# References

```
http://sbml.org/documents/
```

SBase-class 43

SBase-class

SBML type "SBase"

# **Description**

The abstract type from which all other SBML types are derived.

#### Instantiation

A virtual Class: No objects may be created from it.

#### **Slots**

metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.

notes: Object of class "character" containing user-readable XHTML notes about an element.

annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.

cvTerms: Object of class "list" containing instances of CVTerm associated with this element.

sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

# Methods

```
annotation signature(object = "SBase"): gets the annotation slot
annotation<- signature(object = "SBase"): sets the annotation slot
metaId signature(object = "SBase"): gets the metaId slot
metaId<- signature(object = "SBase"): sets the metaId slot
notes signature(object = "SBase"): gets the notes slot
notes<- signature(object = "SBase"): sets the notesslot
cvTerms signature(object = "SBase"): gets the cvTerms slot.
cvTerms<- signature(object = "SBase"): sets the cvTerms slot.
sboTerm signature(object = "SBase"): gets the sboTerm slot.
sboTerm<- signature(object = "SBase"): sets the sboTerm slot.</pre>
```

# Author(s)

Michael Lawrence

#### References

http://sbml.org/documents/

44 SBML import

SBML ir	nport
---------	-------

Read in an SBML file (start here)

# **Description**

Read an SBML file into R.

# Usage

# Arguments

filename the name of the SBML file to parse

text a string of SBML text to parse (instead of file)

dom whether to convert directly to the S4 DOM (TRUE, the default) or leave as the

internal SBMLDocument.

strict whether to report warnings in addition to errors or not (FALSE, the default).

schema whether to perform XML schema validation

consistency whether to perform consistency checks; recommended but might cause perfor-

mance deficiencies.

# Value

```
a SBML object, or a SBMLDocument if dom is FALSE.
```

# Author(s)

Michael Lawrence

# Examples

```
# Read an SBML file
file <- system.file("sbml", "GlycolysisLayout.xml", package = "rsbml")
doc <- rsbml_read(file)

# Read an SBML string
string <- paste(readLines(file),collapse="\n")
doc <- rsbml_read(text = string)</pre>
```

SBML-class 45

SBML-class

SBML type "SBML"

# **Description**

The root element of an SBML document. An actual SBML Model may be retrieved from an instance of this class.

#### Instantiation

Objects can be created by calls of the form new("SBML", ...).

#### **Slots**

```
level: Object of class "integer" indicating the level of the SBML standard (currently at 2).
```

ver: Object of class "integer" indicating the version of the level (currently at 2 for level 2).

model: Object of class "Model" the SBML model itself.

metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.

notes: Object of class "character" containing user-readable XHTML notes about an element.

annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.

cvTerms: Object of class "list" containing instances of CVTerm associated with this element.

sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

## **Extends**

Class "SBase", directly.

#### Methods

```
coerce signature(from = "SBMLDocument", to = "SBML"): constructs the S4 object model from
  a low-level libsbml document.
```

coerce signature(from = "SBML", to = "SBMLDocument"): converts the S4 object model to a low-level libsbml document.

**coerce** signature(from = "SBML", to = "graph"): converts the S4 object model to a graph.

**level** signature(object = "SBML"): gets the level slot

level<- signature(object = "SBML"): sets the level slot</pre>

model signature(object = "SBML"): gets the model slot

model<- signature(object = "SBML"): sets the model slot

46 SBMLDocument-class

```
rsbml\_doc signature(model = "SBML"): converts the S4 object model to a low-level libsbml
    document.

rsbml\_write signature(object = "SBML"): writes this document to a file as SBML.

rsbml\_xml signature(object = "SBML"): converts this document to a string as SBML.

rsbml\_graph signature(object = "SBML"): converts this document to a graph object.

rsbml\_check signature(object = "SBML"): perform consistency checks, see rsbml_check.

simulate signature(object = "SBML"): converts this document to an internal SBMLDocument and calls simulate on it.

ver signature(object = "SBML"): gets the ver slot

ver<- signature(object = "SBML"): sets the ver slot</pre>
```

# Author(s)

Michael Lawrence

#### References

http://sbml.org/documents/

# **Examples**

```
# Get a DOM
dom <- rsbml_read(system.file("sbml", "GlycolysisLayout.xml", package = "rsbml"))
# Get the species ID's
sapply(species(model(dom)), id)
# Convert DOM back to a low-level document for checking
doc <- rsbml_doc(dom)
rsbml_check(doc)
# Write a DOM to a file
## Not run: rsbml_write(dom, "my.xml")</pre>
```

SBMLDocument-class

"SBMLDocument" from libsbml

# **Description**

Low-level libsbml document structure.

#### Instantiation

A virtual Class: No objects may be created from it.

SBMLDocument-class 47

#### **Extends**

```
Class "oldClass", directly.
```

#### Methods

rsbml\\_check signature(object = "SBMLDocument"): rsbml\\_check(object, strict = FALSE,
 consistency = TRUE): Check for problems with the document and signal R conditions if any
 errors are detected. If strict is TRUE, libsbml warnings will be emitted as R warnings (these
 are often too pedantic). If consistency is also TRUE, reports problems regarding internal
 model inconsistencies. This can be time consuming.

rsbml\\_dom signature(doc = "SBMLDocument"): Constructs an S4 object model from a libsbml
document.

```
rsbml\_graph signature(doc = "SBMLDocument"): Converts a libsbml document to a graph.
```

**rsbml\\_problems** signature(object = "SBMLDocument"): reports problems encountered during parsing and/or validation.

```
rsbml\write signature(object = "SBMLDocument"): writes this document to a file as SBML.
```

**rsbml**\\_**xml** signature(object = "SBMLDocument"): converts this document to a string as SBML.

simulate signature(object = "SBMLDocument"): simulate(object, nsim = 10, seed, ...): a shortcut for simulating the model in this document using the SBML ODE Solver library. Arguments in ... should match slots of SOSProtocol. See simulate for more details.

# Author(s)

Michael Lawrence

#### References

```
http://sbml.org/documents/
```

# Examples

```
# Read a document into an R DOM
  dom <- rsbml_read(system.file("sbml", "GlycolysisLayout.xml", package
= "rsbml"))

# Convert to a graph
  graph <- rsbml_graph(dom)

# Write it out to a file
  ## Not run: rsbml_write(dom, "my.xml")

# Or convert it to a string of XML
  rsbml_xml(dom)

# Read into external libsbml data structure
  doc <- rsbml_read(system.file("sbml", "GlycolysisLayout.xml", package
= "rsbml"), dom = FALSE)</pre>
```

48 SBMLProblem-class

```
# Convert it explicitly to an S4 DOM
dom <- rsbml_dom(doc)</pre>
```

SBMLProblem-class

**SBMLProblem** 

# **Description**

Represents an exception thrown during SBML parsing.

# **Details**

There are trivial subclasses for fatal errors (SBMLFatal), recoverable errors (SBMLError), warnings (SBMLWarning) and informational messages (SBMLInfo). Errors become R error conditions, warnings become R warning conditions and messages are output via message.

#### **Slots**

line: The "numeric" line number in the SBML file where the problem was detected.

column: Object of class "numeric" column number in the SBML file where the problem was detected.

msg: Object of class "character", a human-readable description of the problem.

# Methods

.condition signature(object = "SBMLProblem"): constructs a condition object representing
the exception.

# Author(s)

Michael Lawrence

# See Also

SBMLProblems, a container for instances of this class.

SBMLProblems-class 49

SBMLProblems-class

**SBMLProblems** 

# **Description**

A class representing errors encountered during parsing of SBML.

#### **Slots**

```
fatals: A list of SBMLFatal instances.
errors: A list of SBMLError instances.
warnings: A list of SBMLWarning instances.
infos: A list of SBMLInfo instances.
```

#### Methods

```
.throw signature(object = "SBMLProblems"): Throws each SBMLProblem in this object.
errors signature(object = "SBMLProblems"): Gets the errors slot.
fatals signature(object = "SBMLProblems"): Gets the fatals slot.
infos signature(object = "SBMLProblems"): Gets the infos slot.
warns signature(object = "SBMLProblems"): Gets the warns slot.
```

#### Author(s)

Michael Lawrence

# See Also

The rsbml\_problems function for obtaining an instance of this class describing any problems encountered during parsing.

```
SimpleSpeciesReference-class

SBML type "SimpleSpeciesReference"
```

# **Description**

Base class for bindings between a Species and a Reaction.

# Instantiation

Objects can be created by calls of the form new("SimpleSpeciesReference", ...).

50 SOSDesign-class

#### Slots

```
id: Object of class "character" uniquely identifying this component.
```

species: Object of class "character" identifying the Species being referenced.

metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.

notes: Object of class "character" containing user-readable XHTML notes about an element.

annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.

cvTerms: Object of class "list" containing instances of CVTerm associated with this element.

sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

#### **Extends**

```
Class "SBase", directly.
```

## Methods

```
id signature(object = "SpeciesGlyph"): gets the id slot
id<- signature(object = "SpeciesGlyph"): sets the id slot
species signature(object = "SpeciesGlyph"): gets the species slot
species<- signature(object = "SpeciesGlyph"): sets the species slot</pre>
```

#### Author(s)

Michael Lawrence

#### References

```
http://sbml.org/documents/
```

SOSDesign-class

SOSDesign

# **Description**

Specifies the reaction names and their parameter settings for each run in a batch experiment. It extends matrix; each column corresponds to a parameter in the model and each row should hold the parameter settings for one run of the experiment.

SOSDesign-class 51

#### **Details**

It is often desirable to explore the state space of a model by adjusting its initial parameter settings. One could do this by modifying the model itself for each experiment, but this class aims to provide a more convenient and systematic means of running experiments in batch, over a range of parameter settings. The results of the experiment will then contain the output from each run, which may then be compared.

The design is specified as a matrix, and each column in the matrix should correspond to a parameter defined in an SBML model. The column names should identify the parameters. These are not to be confused with the simulation parameters specified in SOSProtocol, which control how the simulation is executed. These should be and are designed to be kept constant across the runs.

There are two different types of parameters: global and local (reaction) parameters. Global parameters may correspond to a Species quantity, Compartment size, or model-level Parameter value. These should be identified in the column names by the id of the corresponding SBML element. The element in the reactions slot for one of these parameters should be the empty string.

The second type of parameter specifies the value of a Parameter element within the KineticLaw of a reaction. These should be named by the id of the Parameter. They also should be namespaced by the containing Reaction id, which is stored in the corresponding element of the reactions slot.

# **Objects from the Class**

Objects can be created by calls of the form new("SOSDesign", data, nrow, ncol, byrow, dimnames, ...). This is the same as initializing a matrix.

#### **Slots**

.Data: Object of class "matrix", holding the parameter settings.

reactions: Object of class "character" of length the number of columns, holding the reaction IDs for parameters local to a reaction (i.e. KineticLaw Parameters). For global parameters, the corresponding value should be the empty string.

# **Extends**

```
Class "matrix", from data part. Class "ExperimentDesign", directly. Class "array", by class "matrix", distance 2. Class "structure", by class "matrix", distance 3. Class "vector", by class "matrix", distance 4, with explicit coerce.
```

#### Methods

```
reactions signature(object = "SOSDesign"): gets the reactions slot.
reactions<- signature(object = "SOSDesign"): sets the reactions slot.</pre>
```

#### Author(s)

Michael Lawrence

52 SOSExperiment-class

#### References

See <a href="http://www.tbi.univie.ac.at/~raim/odeSolver/">http://www.tbi.univie.ac.at/~raim/odeSolver/</a> for more information on the SBML ODE Solver library.

#### See Also

SOSExperiment, the container of this class, for configuring and running a simulation.

SOSExperiment-class SOS Experiment

# **Description**

Implementation of Experiment for simulating SBML models using the SOS: (S)BML (O)DE (S)olver library.

#### **Details**

The general workflow for running a simulation:

- 1. Create or import an SBML DOM.
- 2. Customize the model, for example by adding perturbation Events.
- 3. Wrap the SBML DOM in a SOSSubject, e.g. new("SOSSubject", dom).
- 4. Optionally construct a SOSDesign for running the experiment in batch over several sets of model parameter settings.
- 5. Optionally construct a SOSProtocol for specifying the time points and other parameters controlling the simulation.
- 6. Construct an instance of this class that groups the subject, design and protocol.
- 7. Run simulate on the SOSExperiment, optionally specifying the number of iterations and the random seed.
- 8. Analyze the returned SOSResult, perhaps starting by converting it to a time series with as.ts and making some plots.

# **Objects from the Class**

Objects can be created by calls of the form new("SOSExperiment", ...).

#### Slots

protocol: Object of class SOSProtocol, where the simulation parameters are specified.

design: Object of class SOSDesign, specifying model parameters for each run of a batch experiment.

subject: Object of class SOSSubject, containing the Model to be simulated.

result: Object of class SOSResult containing the result of the simulation.

SOSProtocol-class 53

#### **Extends**

Class Experiment, directly.

#### Methods

simulate signature(object = "SOSExperiment"): simulate(object, nsim = 10, seed, ...): Simulates the SBML document in the subject slot according to the design points in design and parameters in protocol for nsim iterations, using seed as the random seed. Returns an instance of SOSExperiment, which now should include a SOSResult for analysis.

# Author(s)

Michael Lawrence

#### References

See <a href="http://www.tbi.univie.ac.at/~raim/odeSolver/">http://www.tbi.univie.ac.at/~raim/odeSolver/</a> for more information on the SBML ODE Solver library.

# See Also

The simulate method on SBMLDocument is a shortcut, but most users will probably find the above approach most useful.

SOSProtocol-class

SOSProtocol

# **Description**

Holds the parameters controlling the execution of the simulation using the SBML ODE Solver library.

# **Details**

Most users will probably set only the times slot, either directly or through the timeStep slot and the nsim parameter to simulate.

# **Objects from the Class**

Objects can be created by calls of the form new("SOSProtocol", ...). Each argument in ... should correspond to one of the slots described below.

54 SOSProtocol-class

#### Slots

times: A "numeric" vector indicating the time points at which to evaluate the model. Defaults to tail(seq(0, by = timeStep, length.out = nsim + 1), -1). The model is always evaluated at t = 0. This slot is ignored when indefinite (below) is TRUE.

- timeStep: A scalar "numeric" value, giving the length in time between model evaluations. This is used when calculating the default value of times, above, but is otherwise only relevant when the indefinite slot, below, is TRUE. Defaults to 1.
- indefinite: A scalar "logical", indicating whether the simulation should run indefinitely, i.e. until one of the stopping conditions is met. See haltOnEvent and haltOnSteadyState below. Defaults to FALSE.
- atol: Scalar "numeric", the absolute tolerance in integration error. Defaults to 1e-18.
- rtol: Scalar "numeric", the relative tolerance in integration error. Defaults to 1e-10.
- maxStep: Sclar "numeric", the maximum number of steps for integration. Not to be confused with timeStep, etc, above, which control the simulation time points. Defaults to 10000.
- odeMethod: Scalar "character" naming the method for solving ODEs. Either "bdf" (the default) or "adams-moulton".
- iterMethod: Scalar "character", naming the iteration method used by the ODE solver, either "newton" (the default) or "functional".
- maxOrder: Scalar "numeric" indicating maximum order for the ODE solver. Defaults to 5.
- sensMethod: Scalar "character" naming the method for sensitivity analysis. One of "none" (the default and currently the only valid option), "simultaneous", "staggered" or "staggered1".
- haltOnEvent: Scalar "logical" indicating whether the simulation should halt when the model emits an Event. This allows the model to stop the simulation when some state is reached. Defaults to FALSE.
- haltOnSteadyState: Scalar "logical", indicating whether to halt when a steady state is detected. Defaults to FALSE.
- useJacobian: Scalar "logical" indicating whether to use Jacobian ASTs (TRUE, the default) or the internal approximation in the CVODES library.
- storeResults: Scalar "logical" indicating whether to store the entire time course (TRUE, the default) or just the last time point. Just for performance.

#### **Extends**

Class "ExperimentProtocol", directly.

#### Methods

No methods defined with class "SOSProtocol" in the signature.

#### Author(s)

Michael Lawrence

SOSResult-class 55

#### References

See <a href="http://www.tbi.univie.ac.at/~raim/odeSolver/">http://www.tbi.univie.ac.at/~raim/odeSolver/</a> for more information on the SBML ODE Solver library.

#### See Also

The SOSExperiment class, which contains a SOSProtocol instance, for setting up and running a simulation.

SOSResult-class

SOSResult

# **Description**

A result from simulating an SOSExperiment. Contains the time course for each of the model variables: the Species quantities, Compartment sizes, Parameter values, and Reaction rates.

#### Slots

data: A "data. frame" containing the time course data. Each row contains the value at a single time point for a single time course. Has the following columns:

sample A factor, the run number, only exists if there were multiple runs, see SOSDesign.

type A factor, the SBML element type for the time course, e.g. "species".

id A factor, the id of the SBML element for the time course.

time The numeric time value for the time point.

value The actual numeric value for the time course at that time.

sens: A "matrix" with results from sensitivity analysis, not yet supported.

# Extends

Class "ExperimentResult", directly.

#### Methods

**as.ts** signature(x = "SOSResult"): converts this object to a time course object of class ts. This allows analysis of the results with existing R infrastructure for time course analysis.

compartments signature(object = "SOSResult"): returns a subset containing only the Compartment
size courses.

parameters signature(object = "SOSResult"): returns a subset containing only the global Parameter
 value courses.

**reactions** signature(object = "SOSResult"): returns a subset containing only the Reaction rate courses.

species signature(object = "SOSResult"): returns a subset containing only the Species quantity courses. 56 SOSSubject-class

# Author(s)

Michael Lawrence

#### References

See <a href="http://www.tbi.univie.ac.at/~raim/odeSolver/">http://www.tbi.univie.ac.at/~raim/odeSolver/</a> for more information on the SBML ODE Solver library.

# See Also

SOSExperiment for running a simulation and obtaining an instance of this class.

SOSSubject-class

SOSSubject

# **Description**

This just marks an SBML object as being a valid subject for simulation using the SBML ODE Solver library.

# **Objects from the Class**

Normally created from a SBML with: new("SOSSubject", model).

# **Extends**

Class "ExperimentSubject", directly. Class "SBML", directly. Class "SBase", by class "SBML", distance 2. Class "Describable", by class "SBML", distance 3.

# Author(s)

Michael Lawrence

## References

See <a href="http://www.tbi.univie.ac.at/~raim/odeSolver/">http://www.tbi.univie.ac.at/~raim/odeSolver/</a> for more information on the SBML ODE Solver library.

#### See Also

SOSExperiment for running a simulation on a SOSSubject.

Species-class 57

Species-class

SBML type "Species"

## **Description**

A participant in an SBML model.

#### Instantiation

Objects can be created by calls of the form new("Species", ...).

#### Slots

id: Object of class "character" uniquely identifying this component.

name: Object of class "character" naming this component.

compartment: Object of class "character" identifying the compartment in which this species is located.

initial Amount: Object of class "numeric" indicating the initial amount for this species (mutually exclusive with initial Concentration).

initialConcentration: Object of class "numeric" indicating the initial concentration for this species (mutually exclusive with initialAmount).

substanceUnits: Object of class "character" identifying the units for the amount of this species or the numerator of the concentration.

spatialSizeUnits: Object of class "character" identifying the units for the denominator of the species concentration.

hasOnlySubstanceUnits: Object of class "logical" indicating whether the quantity of this species is specified as an amount or a concentration.

boundaryCondition: Object of class "logical". If TRUE, indicates that the quantity of this species cannot be changed by a reaction.

charge: Object of class "integer" indicating the electrical charge of this species.

constant: Object of class "logical" indicating whether the quantity of this species can change.

units: Object of class "character", deprecated.

metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.

notes: Object of class "character" containing user-readable XHTML notes about an element.

annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.

cvTerms: Object of class "list" containing instances of CVTerm associated with this element.

sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

58 Species-class

#### **Extends**

```
Class "SBase", directly.
```

#### Methods

```
id signature(object = "Species"): gets the id slot
id<- signature(object = "Species"): sets the id slot</pre>
name signature(object = "Species"): gets the name slot
name<- signature(object = "Species"): sets the name slot</pre>
boundaryCondition signature(object = "Species"): gets the boundaryCondition slot
boundaryCondition<- signature(object = "Species"): sets the boundaryCondition slot
charge signature(object = "Species"): gets the charge slot
charge<- signature(object = "Species"): sets the charge slot</pre>
compartment signature(object = "Species"): gets the compartment slot
compartment<- signature(object = "Species"): sets the compartment slot</pre>
constant signature(object = "Species"): gets the constant slot
constant<- signature(object = "Species"): sets the constant slot</pre>
units signature(object = "Species"): gets the constant slot
units<- signature(object = "Species"): sets the constant slot</pre>
hasOnlySubstanceUnits signature(object = "Species"): gets the hasOnlySubstanceUnits
hasOnlySubstanceUnits<- signature(object = "Species"): sets the hasOnlySubstanceUnits
initialAmount signature(object = "Species"): gets the initialAmount slot
initialAmount<- signature(object = "Species"): sets the initialAmount slot</pre>
initialConcentration signature(object = "Species"): gets the initialConcentration slot
initialConcentration<- signature(object = "Species"): sets the initialConcentration slot</pre>
spatialSizeUnits signature(object = "Species"): gets the spatialSizeUnits slot
spatialSizeUnits<- signature(object = "Species"): sets the spatialSizeUnits slot</pre>
substanceUnits signature(object = "Species"): gets the substanceUnits slot
substanceUnits<- signature(object = "Species"): sets the substanceUnits slot</pre>
```

## Author(s)

Michael Lawrence

## References

```
http://sbml.org/documents/
```

```
SpeciesConcentrationRule-class
```

SBML type "SpeciesConcentrationRule"

# **Description**

**Obsolete** type of rule that describes the concentration of Species.

# Instantiation

Objects can be created by calls of the form new("SpeciesConcentrationRule", ...).

#### Slots

```
species: Object of class "character" identifying the Species. variable: Object of class "character", ignored.
```

type: Object of class "character", deprecated.

math: Object of class "expression" specifying the equation.

metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.

notes: Object of class "character" containing user-readable XHTML notes about an element.

annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.

cvTerms: Object of class "list" containing instances of CVTerm associated with this element. sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

#### **Extends**

Class "AssignmentRule", directly. Class "Rule", by class "AssignmentRule", distance 2. Class "SBase", by class "AssignmentRule", distance 3.

## Methods

```
species signature(object = "SpeciesConcentrationRule"): gets the species slot
species<- signature(object = "SpeciesConcentrationRule"): sets the species slot</pre>
```

#### Author(s)

Michael Lawrence

# References

```
http://sbml.org/documents/
```

60 SpeciesGlyph-class

SpeciesGlyph-class SB/

SBML type "SpeciesGlyph"

# **Description**

A glyph representing a Species in an SBML layout.

# Instantiation

Objects can be created by calls of the form new("SpeciesGlyph", ...).

#### **Slots**

species: Object of class "character" identifying the species this glyph represents.

id: Object of class "character" uniquely identifying this component.

boundingBox: Object of class "BoundingBox" describing the position and size of the graphical object.

metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.

notes: Object of class "character" containing user-readable XHTML notes about an element.

annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.

cvTerms: Object of class "list" containing instances of CVTerm associated with this element.

sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

# **Extends**

Class "GraphicalObject", directly. Class "SBase", by class "GraphicalObject", distance 2.

# Methods

```
species signature(object = "SpeciesGlyph"): gets the species slot
species<- signature(object = "SpeciesGlyph"): sets the species slot</pre>
```

## Author(s)

Michael Lawrence

# References

http://projects.villa-bosch.de/bcb/sbml

SpeciesReference-class 61

```
SpeciesReference-class
```

SBML type "SpeciesReference"

# **Description**

Binds a reactant or product Species to a Reaction.

#### Instantiation

Objects can be created by calls of the form new("SpeciesReference", ...).

#### **Slots**

stoichiometry: Object of class "numeric" indicating the (static) stoichiometric coefficient.

stoichiometryMath: Object of class "StoichiometryMath" that dynamically calculates the stoichiometric coefficient.

id: Object of class "character" uniquely identifying this component.

species: Object of class "character" identifying the Species being referenced.

metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.

notes: Object of class "character" containing user-readable XHTML notes about an element.

annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.

cvTerms: Object of class "list" containing instances of CVTerm associated with this element.

sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

## **Extends**

Class "SimpleSpeciesReference", directly. Class "SBase", by class "SimpleSpeciesReference", distance 2.

# Methods

## Author(s)

Michael Lawrence

#### References

```
http://sbml.org/documents/
```

SpeciesReferenceGlyph-class

SBML type "SpeciesReferenceGlyph"

# **Description**

A glyph representing a SpeciesReference in an SBML layout.

#### Instantiation

Objects can be created by calls of the form new("SpeciesReferenceGlyph", ...).

#### Slots

speciesGlyph: Object of class "character" identifying the SpeciesGlyph representing the Species that is referenced by the underlying SpeciesReference.

speciesReference: Object of class "character" identifying the linkS4class{SpeciesReference} represented by this glyph.

role: Object of class "character" indicating how this glyph should represent the "role" of the underlying SpeciesReference.

glyphCurve: Object of class "Curve" describing this glyph as a curve (optional).

id: Object of class "character" uniquely identifying this component.

boundingBox: Object of class "BoundingBox" describing the position and size of the graphical object.

metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.

notes: Object of class "character" containing user-readable XHTML notes about an element.

annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.

cvTerms: Object of class "list" containing instances of CVTerm associated with this element.

sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

# Extends

Class "GraphicalObject", directly. Class "SBase", by class "GraphicalObject", distance 2.

SpeciesType-class 63

#### Methods

#### Author(s)

Michael Lawrence

#### References

http://projects.villa-bosch.de/bcb/sbml

SpeciesType-class SBML Type "SpeciesType"

# Description

A Species represents a pool of a chemical in a particular linkS4class{Compartment}. This element specifies a type of species, that is, the chemical independent of location.

#### **Objects from the Class**

Objects can be created by calls of the form new("SpeciesType", ...).

## Slots

id: Object of class "character" uniquely identifying this component.

name: Object of class "character" naming this component.

metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.

notes: Object of class "character" containing user-readable XHTML notes about an element.

annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.

cvTerms: Object of class "list" containing instances of CVTerm associated with this element. sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

# **Extends**

```
Class "SBase", directly.
```

#### Methods

```
id signature(object = "SpeciesType"): gets the id slot
id<- signature(object = "SpeciesType"): sets the id slot
name signature(object = "SpeciesType"): gets the name slot
name<- signature(object = "SpeciesType"): sets the name slot</pre>
```

### Note

Requires libsbml >= 3.0

# Author(s)

Michael Lawrence

#### References

```
http://sbml.org/documents/
```

## See Also

**Species** 

StoichiometryMath-class

SBML type "StoichiometryMath"

# **Description**

Dynamically defines the stoichiometry of a SpeciesReference.

# Instantiation

Objects can be created by calls of the form new("StoichiometryMath", ...).

## **Slots**

math: Object of class "expression" that evaluates to the stoichiometric coefficient.

metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.

notes: Object of class "character" containing user-readable XHTML notes about an element.

TextGlyph-class 65

annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.

cvTerms: Object of class "list" containing instances of CVTerm associated with this element.

sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

## **Extends**

```
Class "SBase", directly.
```

#### Methods

```
math signature(object = "StoichiometryMath"): gets the math slot
math<- signature(object = "StoichiometryMath"): sets the math slot</pre>
```

# Author(s)

Michael Lawrence

#### References

```
http://sbml.org/documents/
```

TextGlyph-class

SBML type "TextGlyph"

# Description

A run of text in an SBML layout.

## Instantiation

Objects can be created by calls of the form new("TextGlyph", ...).

# **Slots**

graphicalObject: Object of class "character" identifying the GraphicalObject that this glyph labels (optional).

text: Object of class "character" containing the text shown by the glyph (mutually exclusive with originOfText).

originOfText: Object of class "character" identifying an SBML component whose name is used as the text (mutually exclusive with text).

id: Object of class "character" uniquely identifying this component.

boundingBox: Object of class "BoundingBox" describing the position and size of the graphical object.

66 Trigger-class

metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.

notes: Object of class "character" containing user-readable XHTML notes about an element.

annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.

cvTerms: Object of class "list" containing instances of CVTerm associated with this element. sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

#### **Extends**

Class "GraphicalObject", directly. Class "SBase", by class "GraphicalObject", distance 2.

#### Methods

```
graphicalObject signature(object = "TextGlyph"): gets the graphicalObject slot
graphicalObject<- signature(object = "TextGlyph"): sets the graphicalObject slot
originOfText signature(object = "TextGlyph"): gets the originOfText slot
originOfText<- signature(object = "TextGlyph"): sets the originOfText slot
text signature(x = "TextGlyph"): ...
text<- signature(object = "TextGlyph"): sets the text slot</pre>
```

# Author(s)

Michael Lawrence

# References

http://projects.villa-bosch.de/bcb/sbml

Trigger-class

SBML Type "Trigger"

# Description

Expresses when an Event should be fired.

# **Objects from the Class**

Objects can be created by calls of the form new("Trigger", ...).

Trigger-class 67

# **Slots**

math: Object of class "expression" that evaluates to TRUE when the event should be fired.

metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.

notes: Object of class "character" containing user-readable XHTML notes about an element.

annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.

cvTerms: Object of class "list" containing instances of CVTerm associated with this element.

sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

# **Extends**

```
Class "SBase", directly.
```

#### Methods

```
math signature(domain = "Trigger"): gets the math slot.
math<- signature(object = "Trigger"): sets the math slot.</pre>
```

# Note

Requires libsbml >= 3.0

# Author(s)

Michael Lawrence

#### References

```
http://sbml.org/documents/
```

## See Also

Event, the parent of this element.

68 Unit-class

Unit-class

SBML type "Unit"

# **Description**

A (possibly transformed) reference to a base UnitKind. The transformation is of the form: \$multiplier \* 10^scale \* x^exponent + offset\$.

#### Instantiation

Objects can be created by calls of the form new("Unit", ...).

#### Slots

kind: Object of class "character" identifying a an SBML UnitKind. For possible values see Table 2 in the SBML specification.

exponent: Object of class "integer" indicating the exponent to use in the transformation.

unitScale: Object of class "integer" indicating the order of magnitude of the scaling to use in the transformation.

multiplier: Object of class "numeric" indicating the factor to use for scaling in the transformation.

offset: Object of class "numeric" indicating the amount of constant shift in the transformation.

metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.

notes: Object of class "character" containing user-readable XHTML notes about an element.

annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.

cvTerms: Object of class "list" containing instances of CVTerm associated with this element.

sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

#### **Extends**

```
Class "SBase", directly.
```

## Methods

```
exponent signature(object = "Unit"): gets the exponent slot
exponent<- signature(object = "Unit"): sets the exponent slot
kind signature(object = "Unit"): gets the kind slot
kind<- signature(object = "Unit"): sets the kind slot
multiplier signature(object = "Unit"): gets the multiplier slot</pre>
```

UnitDefinition-class 69

```
multiplier<- signature(object = "Unit"): sets the multiplier slot
offset signature(object = "Unit"): gets the offset slot
offset<- signature(object = "Unit"): sets the offset slot
unitScale signature(x = "Unit"): ...
unitScale<- signature(object = "Unit"): sets the unitScale slot</pre>
```

## Author(s)

Michael Lawrence

#### References

```
http://sbml.org/documents/
```

```
UnitDefinition-class SBML type "UnitDefinition"
```

# **Description**

Associates one or more Units with an ID and name.

#### Instantiation

Objects can be created by calls of the form new("UnitDefinition", ...).

#### Slots

id: Object of class "character" uniquely identifying this component.

name: Object of class "character" naming this component.

units: Object of class "list" containing equivalent Units that are all associated with the same ID and name.

metald: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.

notes: Object of class "character" containing user-readable XHTML notes about an element.

annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.

cvTerms: Object of class "list" containing instances of CVTerm associated with this element. sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

# Extends

```
Class "SBase", directly.
```

70 UnitDefinition-class

# Methods

```
id signature(object = "UnitDefinition"): gets the id slot
id<- signature(object = "UnitDefinition"): sets the id slot
name signature(object = "UnitDefinition"): gets the name slot
name<- signature(object = "UnitDefinition"): sets the name slot
units signature(object = "UnitDefinition"): gets the units slot
units<- signature(object = "UnitDefinition"): sets the units slot</pre>
```

# Author(s)

Michael Lawrence

# References

http://sbml.org/documents/

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